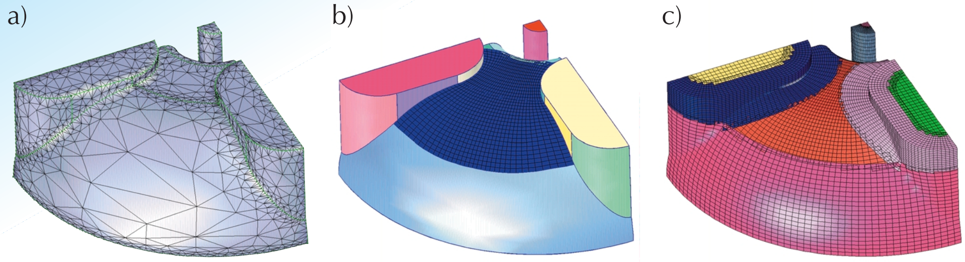
CASC

Center for Applied Scientific Computing

Enabling Computational Technologies for Terascale Simulations



CASC's Rapsodi project is developing rapid setup technology for mesh-based scientific simulations. An intermediate reference triangularization (A) is automatically constructed on the complex surface description from a CAD package and used in the surface mesh generation process (B). The original CAD description spline patches are indicated with different colors in (B). From the resulting set of surface meshes, a volume mesh for the interior of this linear accelerator component can then be constructed (C). Overlapping volume meshes like these can be used with simulation codes developed by CASC's Overture project.

Mission

The Center for Applied Scientific Computing (CASC) at Lawrence Livermore National Laboratory (LLNL) conducts collaborative scientific investigations that utilize the power of high-performance computers and the efficiency of modern computational methods.

Research and development activities are applications-driven and focus on Department of Energy programmatic objectives that require advanced computational technologies. Core competencies include high-performance computing, numerical mathematics, computational physics, algorithm development, and scientific data management and visualization.

LLNL participates in the national Advanced Simulation and Computing program (ASCI) by hosting the ASCI White and ASCI Blue–Pacific massively parallel computers. CASC personnel provide specialized expertise in computer science and computational mathematics to assist Laboratory scientists in developing accurate, reliable terascale scientific simulations. CASC personnel also participate in the national Scientific Discovery through Advanced Computation (SciDAC) program through algorithm research and code development for six of the SciDAC national Integrated Software Infrastructure Centers (ISICs) and through collaborations with many of the SciDAC application projects.

CASC was formed at LLNL in March 1996 as the center for computational science research within the LLNL Computation Directorate. More than 120 numerical mathematicians, computational physicists, and computer scientists in CASC work closely with colleagues in the Computation Directorate, and in Laboratory programs to enable terascale scientific simulations in a variety of application areas.

Specialized Expertise

Within CASC, two-dozen project teams develop new scientific application codes for high-performance computers and apply these codes to collaborative, multidisciplinary scientific investigations. CASC personnel also incorporate new computational technologies into existing scientific codes and refine scientific visualization technologies for select applications. The design, implementation, and evaluation of new computing technologies are critical to the continued success of LLNL's computational science efforts.

CASC conducts research in computer science, scientific data exploration, computational mathematics, computational frameworks, component technologies, and scientific computing applications. Specialists advance superior methods and technologies for terascale computing and collaborate with other scientists to apply them to LLNL, ASCI, and SciDAC simulation codes.

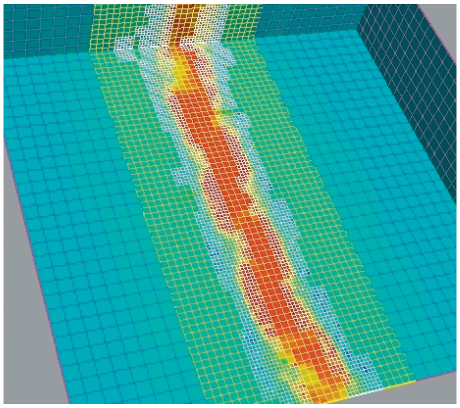
Collaborative Scientific Investigations

CASC researchers collaborate with several LLNL programs on applications in defense, energy, engineering, and environmental sciences. For example, CASC scientists team with other researchers to explore numerical materials properties and turbulent flow in support of the nation's nuclear stockpile stewardship mission (one portion of the ASCI endeavor). Other CASC investigators apply their expertise to challenges in data warehousing. Complex simulation codes are applied to study environmental issues using global climate modeling. First Principles Molecular Dynamics simulations have provided very significant improvement to understanding shock propagation in liquid deuterium. And the Sapphire project aims to improve data management and pattern recognition.

In order to improve memory system performance, CASC is exploring dynamic access optimizations-run-time techniques that use memory system hardware more efficiently by altering the order or apparent location of memory accesses without changing their results. CASC researchers are developing computer codes that simulate propagation and interaction of electromagnetic fields. Each of these collaborative scientific investigations requires high-performance computing and state-of-the-art numerical methods.

Enabling Computational Technologies

Terascale scientific simulations demand scalable numerical methods



In this hybrid continuum-particle simulation, SAMR concentrates particles to resolve mixing of two gasses. Particles exist only in the finest cells (white boundaries).

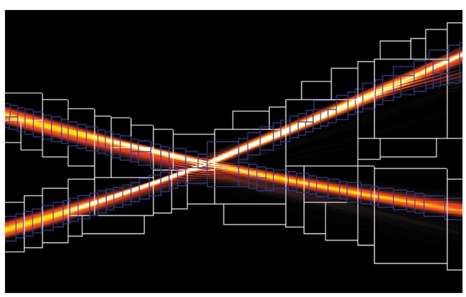
and flexible code frameworks. CASC research excels in both areas. Recent research produced a fast and scalable multigrid preconditioned conjugate gradient solver that substantially improves performance on difficult implicit systems. Current work with ASCI code groups has modified this technology for application to radiation-diffusion problems. In the area of code frameworks, CASC earns international recognition for its parallel structured adaptive mesh refinement (SAMR) code infrastructure, which is used for multi-scale simulations and in applications such as laser-plasma interactions. CASC's Rapsodi project is developing rapid setup technology for mesh-based scientific simulations. A thorough understanding of the performance of various parallel programming methods is critical to all these efforts.

Institute for Scientific Computing Research

The mission of the Institute for Scientific Computing Research (ISCR) is to foster collaborations between LLNL and academic researchers in the areas of scientific computing, computer science, and computational mathematics.

The ISCR is jointly administered by the LLNL's University Relations Program (URP) and CASC, and this joint relationship also expresses its mission. The ISCR is the administrative host and technical matchmaker for several dozen summer or year-round graduate students, post-doctoral fellows, and visiting faculty. The ISCR also has substantial collaborations with UC researchers that take place on UC campuses as well as in residence at the Lab. Many of these research collaborations are centered on the Laboratory's unique computational facilities, which include the world's most powerful general-purpose scientific supercomputer.

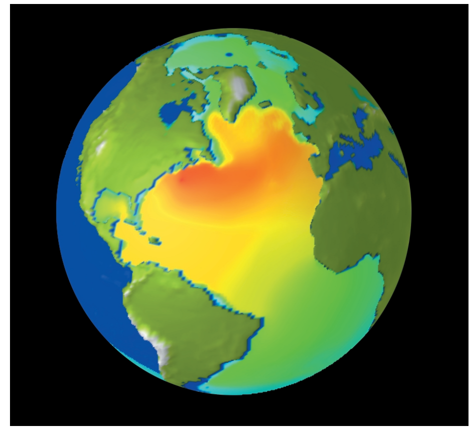
The ISCR also administers the university portion of the ASCI Institute for Terascale Simulation (ITS) at LLNL, which sponsors technical workshops and short courses, a distinguished lecturer series, and summer tutorials for graduate students. An extensive externally networked ISCR cost-effectively expands the level and scope of national computational science expertise available to the Laboratory, while disseminating the Laboratory's own contributions to the national community.



Adaptive mesh calculation of a filamenting beam.

Computing Resources

The Laboratory hosts ASCI White, an ultra-computer configured with 8,192 microprocessors in 512 shared-memory nodes with high-bandwidth, low-latency interconnectivity. Each node consists of 16 Power3-II CPUs with IBM's latest semi-conductor technology (silicon-on-insulator and



Simulation of ocean carbon dioxide concentration resulting from injection near New York City.

copper interconnects). Its 8 terabyte-memory is about 125,000 times that of a 64-MB PC. ASCI White holds 160 terabytes of storage space in about 7,000 disk drives, approximately 16,000 times the storage capacity of a desktop computer with a 10-GB hard drive. An additional IBM system of 1,464 four-processor nodes has an aggregate of 2.6 TB of memory and is rated at 3.9 TeraFLOPs of peak performance. LLNL has also collaborated with Compaq to deploy several clusters of Alpha-based SMPs as part of the Laboratory's Multiprogram-matic and Institutional Computing Initiative. One configuration boasts peak performance of more than 70 GigaFLOPs and 56 GB of memory. Visualization expertise is available through the Computation Directorate's Visualization Laboratory and a variety of power wall display systems.

For additional information on the many facets of CASC's research efforts, visit the Web site at http://www.llnl.gov/CASC.

If you are interested in a career, post-doctoral, or visiting position, please contact Steven Ashby, Founding Director, sfashby@llnl.gov, or Peter Eltgroth, peltgroth@llnl.gov.

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